

A Schroedinger link between non-equilibrium thermodynamics and Fisher information

B. R. Frieden¹, A. Plastino^{1,2,3}, A. R. Plastino^{2,3}, and B. H. Soffer^{1,4}

¹*University of Arizona at Tucson*

²*Universidad Nacional de La Plata,*

C.C. 727, 1900 La Plata, Argentina

³*Argentine National Research Center (CONICET)*

⁴*Postal address: 665 Bienvenida Avenue, Pacific Palisades,*

California 90272

Abstract

It is known that equilibrium thermodynamics can be deduced from a constrained Fisher information extremizing process. We show here that, more generally, both non-equilibrium and equilibrium thermodynamics can be obtained from such a Fisher treatment. Equilibrium thermodynamics corresponds to the ground state solution, and non-equilibrium thermodynamics corresponds to excited state solutions, of a Schroedinger wave equation (SWE). That equation appears as an output of the constrained variational process that extremizes Fisher information. Both equilibrium- and non-equilibrium situations can thereby be tackled by one formalism that clearly exhibits the fact that thermodynamics and quantum mechanics can both be expressed in terms of a formal SWE, out of a common informational basis.

PACS. numbers: 05.45+b, 05.30-d

I. INTRODUCTION

The information content of a normalized probability distribution $P(i), i = 1, \dots, N$, where the index i runs over the states of the system one is trying to study, is given by Shannon's information measure (IM) [1]

$$S = - \sum_{i=1}^N P(i) \ln[P(i)]. \quad (1)$$

The choice of the logarithmic base fixes the information units. If the basis is 2 then S is measured in *bits*. If one chooses Boltzmann's constant as the informational unit and identifies Shannon's IM with the thermodynamic entropy, then the whole of statistical mechanics can be elegantly reformulated by extremization of Shannon's S , subject to the constraints imposed by the *a priori* information one may possess concerning the system of interest [1].

Now, the phenomenal success of thermodynamics and statistical physics crucially depends upon certain necessary mathematical relationships involving energy and entropy (Legendre transform structure). In the *equilibrium situation* these relationships are also valid if one replaces S by Fisher's information measure I (FIM) [2]. Using this measure [3], the entire Legendre-transform structure of thermodynamics can be re-expressed (i.e., I replaces Boltzmann-Shannon S). In general, this abstract Legendre structure constitutes an essential ingredient that allows one to build up a statistical mechanics. Fisher information I allows then for such a construction. Also, a desired concavity property, obeyed by I , further demonstrates its utility as a statistical mechanics generator.

Here we will show that the variational treatment of Fisher information also accounts for *non-equilibrium situations*. We will *connect* Fisher information I with non-equilibrium thermodynamics via the Schroedinger equation (SWE). Such a connection is of interest because it clearly shows that equilibrium and non-equilibrium states have a common informational origin that is expressed by the SWE. The same SWE also allows for quantum scenarios, or even mixed quantum and thermodynamic scenarios.

The interested reader might want to consult works by Frieden, Soffer, Nikolov, Plastino, Silver, Hughes, Reginatto, Hall, and others, that have shed much light upon the manifold

physical applications of Fisher’s information measure [4–17]. Frieden and Soffer have shown that FIM provides one with a powerful variational principle that yields the canonical Lagrangians of theoretical physics [11]. Additionally, I has been shown to characterize an “arrow of time” with reference to the celebrated Fokker-Planck equation [15–17,20,21].

II. FISHER’S INFORMATION MEASURE FOR TRANSLATION FAMILIES. A VARIATIONAL TREATMENT

Consider a system that is specified by a physical parameter θ at a given time t . Let $g(x, \theta|t)$ describe the probability density function (PD) for this parameter at that time. Of course, by normalization,

$$\int dx g(x, \theta|t) = 1. \quad (2)$$

The Fisher information measure (FIM) I is of the form

$$I = \int dx g \left[\frac{\partial g / \partial \theta}{g} \right]^2, \quad g = g(x, \theta|t). \quad (3)$$

The special case of *translation families* is of use. These are mono-parametric families of distributions of the form

$$g(x, \theta|t) = p(u|t), \quad u \equiv x - \theta, \quad (4)$$

which are known up to the shift parameter θ . Following Mach’s principle, all members of the family possess identical shape $p(u|t)$ (there are no absolute origins). Here FIM takes the appearance [21]

$$I = \int dx \frac{(\partial p / \partial x)^2}{p}, \quad p = p(x|t). \quad (5)$$

Our present considerations assume one is dealing with coordinates x that belong to \mathcal{R} . Let us focus attention upon the positive-definite, normalized PDF $p(x|t)$, evaluated at the time t . It of course obeys normalization

$$\int dx p(x|t) = 1. \quad (6)$$

Let the mean values

$$\theta_k \equiv \langle A_k \rangle \text{ of } M \text{ functions } A_k(x), \quad k = 1, \dots, M \quad (7)$$

be measured at the time t . By definition

$$\langle A_k \rangle_t = \int dx A_k(x) p(x|t), \quad k = 1, \dots, M. \quad (8)$$

These mean values will play the role of thermodynamical variables, as explained in [2].

It is of importance to note that the prior knowledge (8) *represents information at the fixed time t* . The problem we attack is to find the PDF $p \equiv p_{MFI}$ that extremizes I subject to prior conditions (6)-(7). Our Fisher based extremization problem takes the form

$$\delta_p \{ I(p) - \alpha \langle 1 \rangle - \sum_k^M \lambda_k \langle A_k \rangle_t \} = 0, \quad p \equiv p(x|t), \quad (9)$$

at the given time t . Eq. (9) is equivalent to

$$\delta_p \left\{ \int dx \left(F_{Fisher}(p) - \alpha f - \sum_k^M \lambda_k A_k p \right) \right\} = 0, \quad (10)$$

where we have introduced the $(M+1)$ Lagrange multipliers $(\alpha, \lambda_1 \dots \lambda_M)$, where each Lagrange multiplier $\lambda_k \equiv \lambda_k(t)$. Variation leads now to

$$\int dx \delta p \left\{ (p)^{-2} \left(\frac{\partial p}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left[(2/p) \frac{\partial p}{\partial x} \right] + \alpha + \sum_k^M \lambda_k A_k \right\} = 0, \quad (11)$$

and, on account of the arbitrariness of δp

$$\left\{ (p)^{-2} \left(\frac{\partial p}{\partial x} \right)^2 + \frac{\partial}{\partial x} \left[(2/p) \frac{\partial p}{\partial x} \right] + \alpha + \sum_k^M \lambda_k A_k \right\} = 0. \quad (12)$$

It is clear that the normalization condition on p makes α a function of the λ_i 's. Let then $p_I(x, \{\lambda\})$ be a solution of (12), where obviously, $\{\lambda\}$ is an M -dimensioned Lagrange multipliers vector. The extreme Fisher information is now a function of time

$$I = \int dx \frac{(\partial p / \partial x)^2}{p} \equiv I(t), \quad (13)$$

since $p = p(x|t)$. Since p extremized I we write

$$p \equiv p_I, \quad p_I \equiv p_I(x|t).$$

Let us now find the general solution of Eq. (12). For the sake of simplicity let us define

$$G(x, t) = \alpha + \sum_k^M \lambda_k(t) A_k(x), \quad (14)$$

and recast (12) as

$$\left[\frac{\partial \ln p_I}{\partial x}\right]^2 + 2\frac{\partial^2 \ln p_I}{\partial x^2} + G(x) = 0. \quad (15)$$

We introduce now the identification [13] $p_I = (\psi)^2$, recalling that $\psi(x)$ can always be assumed real for one-dimensional problems [2]. Introduce now the new functions

$$v = \frac{\partial \ln \psi}{\partial x}, \quad \psi \equiv \psi(x, t), \quad v \equiv v(x, t). \quad (16)$$

Then (15) simplifies to

$$v' = -\left\{\frac{G}{4} + v^2\right\}, \quad (17)$$

where the prime stands for the derivative with respect to x . The above equation is a Riccati equation [22]. Introduction further of [22]

$$u = \exp\left\{\int^x dx [v]\right\}, u = u(x, t) \quad (18)$$

i.e.,

$$u = \exp\left\{\int^x dx \frac{d \ln \psi}{dx}\right\} = \psi, \quad (19)$$

places (15) in the form of a Schroedinger wave equation (SWE) [22]

$$-(1/2)\psi'' - (1/8)\sum_k^M \lambda_k(t) A_k \psi = \alpha\psi/8, \quad (20)$$

where the Lagrange multiplier $\alpha/8$ plays the role of an energy eigenvalue, and the sum of the $\lambda_k A_k(x)$ is an effective potential function

$$U = (1/8)\sum_k^M \lambda_k(t) A_k, U = U(x, t). \quad (21)$$

Note that no specific potential has been assumed, as is appropriate for thermodynamics. Also, we remark that U is a time-dependent potential function and will permit non-equilibrium solutions. The specific $A_k(x)$ to be used here depend upon the nature of the physical application at hand (cf. Eq. (8)). This application could be of either a classical or a quantum nature.

Also notice that equation (20) represents a boundary value problem, generally with multiple solutions, in contrast with the unique solution one obtains when employing Jaynes-Shannon's entropy in place of FIM [1]. As discussed in some detail in [2], the solution leading to the lowest I -value is the equilibrium one. That was the only solution discussed there. Here we wish to generalize the concomitant discussion and ask: can we choose other solutions?

III. RUMER AND RYVKIN'S APPROACH TO NON-EQUILIBRIUM THERMODYNAMICS

In Ref. [23], Rumer and Ryvkin (R-R) use the conventional Boltzmann transport equation to build up non-equilibrium solutions. They take the following approach:

- Consider a non-equilibrium state of a gas after the lapse of a time t large compared to the time of initial randomization. The time t is regarded as *fixed*.
- The time t is, also, small compared to the macroscopic relaxation time T^* for attaining the Maxwell-Boltzmann law f_0 on velocities.
- At each point of the vessel containing the gas a state arises which is close to the *local* equilibrium state

$$f_0 = \text{Maxwell} - \text{Boltzmann law on velocities.}$$

- This allows one to expand the non-equilibrium distribution $f(x|t)$ as

$$f_0 = 1 + \epsilon\phi(x, t), \quad f_0 \equiv f(x, t) \quad (22)$$

where ϵ is small and the function ϕ is to be the object of our endeavors.

- The unknown function $\phi(x, t)$ may itself be expanded as a series of (orthogonal) Hermite-Gaussian polynomials $H_i(x)$ with coefficients $a_i(t)$ at the fixed time t ,

$$f(x, t) = \sum a_i(t) H_i(x) \quad (23)$$

It is important to remark that Hermite-Gaussian polynomials are orthogonal with respect to a Gaussian kernel, i.e., the *equilibrium distribution*. No other set of functions is orthogonal (and complete) with respect to a Gaussian kernel function.

- Because of orthogonality, the unknown coefficients $a_i(t)$ relate linearly to appropriate (unknown) moments of f over velocity space (x -space).
- Substituting the expansion for f into the transport equation and integrating over all velocities yields now a set of first-order differential equations in the moments (which are generally a function of the fixed time value t).
- These are now solvable subject to *known initial conditions*, like our expectation values. The moments now become known (*including any time dependence*).
- As a consequence the coefficients $a_i(t)$ of (23) are also known, which gives f .

What does the f as determined above represent? According to Ref. [23], the solution of the above system of equations would be equivalent to the exact solution of Boltzmann's equation (if enough a priori information were available).

We emphasize that R-R do not use an SWE in their approach.

IV. CONNECTING THE SWE EXCITED SOLUTIONS TO NON-EQUILIBRIUM THERMODYNAMICS

Returning to our analysis, we ask: Can the excited SWE solutions to Eq. (20) represent non-equilibrium states of thermodynamics [11,21]? In order to answer this question, consider again the case in which x is a velocity and one seeks the non-equilibrium probability $p(x|t)$.

Let excited solutions $\psi_n(x, t)$ to the SWE Eq. (20) be identified by a subindex value $n > 0$. These amplitude functions are superpositions of Hermite-Gaussian polynomials of the form

$$\psi_n(x, t) = \sum_i b_{in}(t) H_i(x), \quad n = 1, 2, \dots \quad (24)$$

The total number of coefficients $b_{ni}(t)$ depends upon how far from equilibrium we are. At equilibrium there is only one such coefficient.

We will show that the squares of these amplitudes agree, under certain conditions (see below), with the known solutions of the Boltzmann transport equation [11,21,23]. Our coefficients $b_{in}(t)$ are computed at the fixed time t at which our input data $\langle A_k \rangle_t$ are collected. While the ground state solution of (20) gives the equilibrium states of thermodynamics [2], the excited solutions of (20) will be shown to be give non-equilibrium states. For this to happen, our functions $\psi_n(x, t)$ will have to be connected to the R-R $f(x, t)$ of Eq. (23) via the squaring operation $\psi_n^2(x, t)$.

Notice that the square of an expansion in Hermite-Gaussians is likewise a superposition of Hermite-Gaussians, with coefficients $c_{in}(t)$

$$\psi_n^2(x, t) = \sum_i c_{in}(t) H_i(x), \quad n = 1, 2, \dots \quad (25)$$

We argue now to the effect that, for fixed n , the R-R coefficients $a_i(t)$ and our $c_{in}(t)$ are equal.

First of all, the R-R coefficients are certainly computed, like ours, at a *fixed* time t . That is, their momenta are evaluated at that time. Likewise ours (the $\langle A_k \rangle$ of (8)) can be regarded as velocity momenta at that time as well.

The difference between the R-R coefficients and ours is one of physical origin, as follows. R-R *solve for* the velocity moments at the fixed time t . These M_{RR} moments are computed using the R-R a_i of Eq. (23). We, instead, collect *as experimental inputs* these velocity moments (at the fixed time t). Thus, if the M_{RR} moments *coincide with our experimental inputs*, necessarily the $a_i(t)$ and the $c_{in}(t)$ have to coincide well. Let us repeat: the R-R moments at the time t are physically correct by construction, since they actually solve for them via use of the Boltzmann transport equation. The premise of our constrained Fisher information approach is that its input constraints (here our velocity moments $\langle A_k \rangle_t$) are correct, since they come *from experiment*. (They calculate, we measure.)

If there is no agreement between the R-R moments and our experimental inputs, two possibilities come to mind: a) we are measuring inputs showing strong quantum effects, while the R-R treatment can not handle such a case (being classical), or b) the number M of available experimental data we use as inputs does not equal the number M_{RR} of R-R computed moments. This possible disagreement is, however, of a logistic rather than fundamental nature.

The required number of expansion coefficients b_i in Eq. (24) is of interest. At equilibrium only one is needed (b_0), as that situation is described by a grand-canonical distribution function that is Gaussian. Next, if the system is sufficiently close to equilibrium then very few are needed. Hence, near-equilibrium cases should pose little numerical difficulty.

Summing up, the approach given in this paper will give exactly the same solutions *at the fixed (but arbitrary) time t as does the R-R approach*. Therefore, for fixed n , our $c_{in}(t)$ s coincide with the R-R $a_i(t)$ s and our $p(x|t)$ coincide with the R-R $f(x, t)$. This holds at each time t (Cf. Eq. (8)). For any other time value, t' , say, we would have to input new $\langle A_k \rangle$ values appropriate for that time. R-R, instead, get coefficients $a_i(t)$ valid for continuous

time t , since they are using Boltzmann's transport equation, which is a continuous one. Our approach, by contrast, yields solutions valid at discrete point of time t . This distinction, "discrete versus continuous", does not compromise the validity of the Fisher- Schroedinger, non-equilibrium thermodynamics bridge that we have built up here.

V. CONCLUSIONS AND DISCUSSION

It is becoming increasingly evident [4–7,11,14,15,20,21] that Fisher information I is vital to the fundamental nature of physics. In a previous effort [2], we showed how the I -concept lays the foundation for a thermodynamics *in the usual equilibrium* case. Here we have shown that *non – equilibrium* thermodynamics case can likewise be formed in this way. This considerably expands the horizon envisioned in [2]

The main result of this work is the establishment, by means of Fisher information, of a connection between non-equilibrium thermodynamics and quantum mechanics. The emphasis here lies in the word "connection". Why would such a link be of interest? Because it clearly shows that thermodynamics and quantum mechanics can both be expressed by a formal SWE (20), out of a common informational basis [21].

The physical meaning of this SWE is flexible, since its "potential function" $U(x)$ originates in data $\langle A_k \rangle_t$, via Eq. (21), of a *physically general* nature. This depends upon the application. The $\langle A_k \rangle_t$ are introduced into the theory as *empirical* inputs. The approach also encompasses quantum effects. In the latter cases the effective potential function includes quantum effects. Also, the Planck constant \hbar , which does not explicitly appear in Eq. (20), would appear in one or more inputs $\langle A_k \rangle_t$ as, for example, would occur if the expectation value of the linear momentum of an electron were measured. The classical Boltzmann equation of the R-R approach would then of course *not* be useable. In this way, our approach encompasses both quantum- and classical thermodynamic effects.

REFERENCES

- [1] E. T. Jaynes in *Statistical Physics*, ed. W. K. Ford (Benjamin, New York, 1963); A. Katz, *Statistical Mechanics*, (Freeman, San Francisco, 1967).
- [2] R. Frieden, A. R. Plastino, A. Plastino, and B. H. Soffer, *Phys. Rev. E* **60**, 48 (1999).
- [3] R. A. Fisher, *Proc. Camb. Soc.* **22**, 700 (1925).
- [4] B. R. Frieden, *Am. J. Phys.* **57**, 1004 (1989).
- [5] B. R. Frieden, *Phys. Lett. A* **169**, 123 (1992).
- [6] B. R. Frieden, in: *Advances in imaging and electron physics* Vol. 90, ed. P.W. Hawkes (Academic, New York, 1994) pp. 123-204.
- [7] B. R. Frieden, *Physica A* **198**, 262 (1993).
- [8] B. R. Frieden and R. J. Hughes, *Phys. Rev. E* **49**, 2644 (1994).
- [9] B. Nikolov and B. R. Frieden, *Phys. Rev. E* **49**, 4815 (1994).
- [10] B. R. Frieden, *Phys. Rev. A* **41**, 4265 (1990).
- [11] B. R. Frieden and B. H. Soffer, *Phys. Rev. E* **52**, 2274 (1995).
- [12] B. R. Frieden, *Founds. Phys.* **21**, 757 (1991).
- [13] R. N. Silver in *E. T. Jaynes: Physics and Probability*, edited by W. T. Grandy, Jr. and P. W. Milonni (Cambridge University Press, Cambridge, 1992).
- [14] A. Plastino, A. R. Plastino, H. G. Miller, and F. C. Khana, *Phys. Lett. A* **221**, 29 (1996).
- [15] A. R. Plastino and A. Plastino, *Phys. Rev. E* **54**, 4423 (1996).
- [16] A. R. Plastino, A. Plastino, and H. G. Miller, *Phys. Rev. E* **56**, 3927 (1997).
- [17] A. Plastino, A. R. Plastino, and H. G. Miller, *Phys. Lett. A* **235**, 129 (1997).

- [18] S. Kullback, *Information theory and statistics* (Wiley, NY, 1959).
- [19] M. Ravicule, M. Casas, and A. Plastino, *Phys. Rev. A* **55** (1997) 1695.
- [20] A. R. Plastino, M. Casas, and A. Plastino, *Phys. Lett. A* **246**, 498 (1998).
- [21] R. Frieden, *Physics from Fisher information* (Cambridge University Press, Cambridge, England, 1998).
- [22] P. I. Richards, *Manual of mathematical physics* (Pergamon Press, London, 1959) p. 342.
- [23] Y. B. Rumer and M. S. Ryvkin, *Thermodynamics, statistical mechanics and kinetics* (MIR Publishers, Moscow, 1980).
- [24] B. R. Frieden and B. H. Soffer, *Found.of Physics* **13**, 89 (2000).